

Factorization of multiple integrals representing the density matrix of a finite segment of the Heisenberg spin chain

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Abstract

We consider the inhomogeneous generalization of the density matrix of a finite segment of length m of the antiferromagnetic Heisenberg chain. It is a function of the temperature T and the external magnetic field h , and further depends on m ‘spectral parameters’ ξ_j . For short segments of length 2 and 3 we decompose the known multiple integrals for the elements of the density matrix into finite sums over products of single integrals. This provides new numerically efficient expressions for the two-point functions of the infinite Heisenberg chain at short distances. It further leads us to conjecture an exponential formula for the density matrix involving only a double Cauchy-type integral in the exponent. We expect this formula to hold for arbitrary m and T but zero magnetic field.

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1 Introduction

The study of correlation functions of solvable quantum systems took a new direction in 1992 when Jimbo et al. [16] shifted the focus of attention from the two-point functions to the density matrix of a sub-system as the object of principal interest. They managed to derive an m -fold integral expression for the density matrix of a chain segment of length m of the infinitely long, antiferromagnetic XXZ -spin- $\frac{1}{2}$ chain in the off-critical regime. In the following years this work was generalized to the critical regime [17], to non-zero magnetic field [18] and, most recently [12, 14], to non-zero magnetic field and temperature.

The above mentioned works have in common that they all deal with an inhomogeneous generalization of the density matrix obtained by placing ‘spectral parameters’ or ‘inhomogeneities’ onto m consecutive vertical lines of the corresponding vertex model. The homogeneous limit, when all the spectral parameters go to zero, is involved and is usually only taken at a late stage of the calculations after all formulae have been transformed into an appropriate form. Moreover, the inhomogeneous density matrix (at zero magnetic field and zero temperature) satisfies a first order difference equation in the inhomogeneities which is part of the novel reduced quantum Knizhnik-Zamolodchikov equation (rqKZ) [2, 3].

In [5, 6] the multiple integrals for a specific zero temperature density matrix element of the isotropic Heisenberg chain were explicitly evaluated for $m = 3$ and $m = 4$. This line of research was further pursued in [7, 20]. In a second line of research representations of the zero temperature density matrix which do not involve multiple integrals were developed starting from functional equations [2, 3, 8–10, 21, 22]. This helped to work out further concrete examples of short-range correlation functions, such that nowadays closed analytic expressions for the ground state spin-spin correlators are known up to the seventh neighbour. In its most elaborate form of the rqKZ equation the functional equations were then used in [1] to derive an exponential formula for the density matrix of a segment of length m of the XXX chain that involves only a double Cauchy-type integral in the exponent. In the recent paper [4] such a formula was obtained for the XXZ and XYZ models as well.

This article is concerned with an attempt to generalize both of the above approaches to finite temperature and partially also to finite magnetic field. We concentrate on the isotropic Heisenberg chain which on a periodic lattice of L sites has the Hamiltonian

$$H = J \sum_{j=1}^L (\sigma_j^\alpha \sigma_{j+1}^\alpha - 1). \quad (1)$$

Here σ_j^α , $\alpha = x, y, z$, acts as a Pauli matrix on site j of the spin chain, and implicit summation over Greek indices is understood. For this model we have achieved a factorization of the density matrix for $m = 2$ and $m = 3$ into single integrals valid for arbitrary finite temperature and finite magnetic field. Based on this result and on results obtained from the high temperature expansion of the multiple integrals [24] we

present a conjecture for a finite temperature generalization of the exponential formula in [1].

The paper is organized as follows. In section 2 we recall the multiple integral formula for the density matrix elements. In section 3 we explain the reduction procedure of those integrals in the cases $m = 2$ and $m = 3$. In section 4 we discuss our conjecture on the exponential form for zero magnetic field. In the appendix we show compact formulae for the density matrix elements for $m = 3$.

2 The multiple integral formula for the density matrix

The density matrix is a means to describe a sub-system as a part of a larger system in thermodynamic equilibrium in terms of the degrees of freedom of the sub-system. In our case the sub-system will consist of m consecutive sites of the spin chain. We first define a ‘statistical operator’ by

$$\rho_L = \exp(-(H - hS^z)/T), \quad (2)$$

where $S^z = \frac{1}{2} \sum_{j=1}^L \sigma_j^z$ is the conserved z -component of the total spin, T is the temperature and h is the homogeneous external magnetic field. In terms of this statistical operator the density matrix of a finite sub-chain of length m of the infinite chain is expressed as

$$D(T|h) = \lim_{L \rightarrow \infty} \frac{\text{tr}_{m+1 \dots L} \rho_L}{\text{tr}_{1 \dots L} \rho_L}. \quad (3)$$

By construction, the thermal average of every operator A acting non-trivially only on sites 1 to m can then be written as

$$\langle A \rangle_{T,h} = \text{tr}_{1 \dots m} A_{1 \dots m} D(T|h), \quad (4)$$

where $A_{1 \dots m}$ is the restriction of A to the first m lattice sites.

The tensor products $e_{\beta_1}^{\alpha_1} \otimes \dots \otimes e_{\beta_m}^{\alpha_m}$ composed of 2×2 matrices e_{β}^{α} , $\alpha, \beta = 1, 2$, with a single non-zero entry at the intersection of row β and column α form a basis of $\text{End}((\mathbb{C}^2)^{\otimes m})$. The matrix elements of the density matrix with respect to this basis can be represented as

$$D_{\beta_1 \dots \beta_m}^{\alpha_1 \dots \alpha_m}(T|h) = \lim_{\xi_1, \dots, \xi_m \rightarrow 0} D_{\beta_1 \dots \beta_m}^{\alpha_1 \dots \alpha_m}(\xi_1, \dots, \xi_m), \quad (5)$$

where the expression under the limit is the inhomogeneous density matrix element mentioned in the introduction. Due to the conservation of S^z it is non-zero only if $\sum_{j=1}^m (\alpha_j - \beta_j) = 0$.

For the non-zero inhomogeneous density matrix elements (5) of the XXZ chain a multiple integral formula was obtained in [12, 14]. When specialized to the isotropic

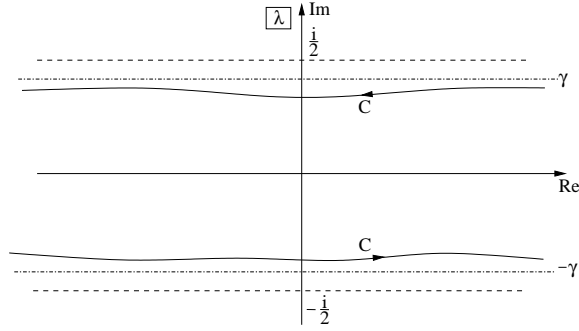


Figure 1: The canonical contour C surrounds the real axis in counterclockwise manner inside the strip $-\frac{1}{2} < \text{Im } \lambda < \frac{1}{2}$.

limit (1) it reads

$$D_{\beta_1 \dots \beta_m}^{\alpha_1 \dots \alpha_m}(\xi_1, \dots, \xi_m) = \left[\prod_{j=1}^{|\alpha^+|} \int_C \frac{d\omega_j}{2\pi(1 + \mathfrak{a}(\omega_j))} \prod_{k=1}^{\tilde{\alpha}_j^+ - 1} (\omega_j - \xi_k - i) \prod_{k=\tilde{\alpha}_j^+ + 1}^m (\omega_j - \xi_k) \right] \\ \left[\prod_{j=|\alpha^+|+1}^m \int_C \frac{d\omega_j}{2\pi(1 + \bar{\mathfrak{a}}(\omega_j))} \prod_{k=1}^{\tilde{\beta}_j^- - 1} (\omega_j - \xi_k + i) \prod_{k=\tilde{\beta}_j^- + 1}^m (\omega_j - \xi_k) \right] \\ \frac{\det G(\omega_j, \xi_k)}{\prod_{1 \leq j < k \leq m} (\xi_k - \xi_j)(\omega_j - \omega_k - i)}. \quad (6)$$

The formula involves certain positive integers $\tilde{\alpha}_j^+$ and $\tilde{\beta}_j^-$ derived from the sequences of indices $(\alpha_n)_{n=1}^m$, $(\beta_n)_{n=1}^m$ specifying the matrix element. The indices take values 1, 2 corresponding to spin-up or spin-down. We shall denote the position of the j -th up-spin in $(\alpha_n)_{n=1}^m$ by α_j^+ and that of the k -th down-spin in $(\beta_n)_{n=1}^m$ by β_k^- . Then, by definition, $\tilde{\alpha}_j^+ = \alpha_{|\alpha^+| - j + 1}^+$, where $|\alpha^+|$ is the number of up-spins in $(\alpha_n)_{n=1}^m$, and $j = 1, \dots, |\alpha^+|$. Similarly $\tilde{\beta}_j^- = \beta_{j - |\alpha^+|}^-$, $j = |\alpha^+| + 1, \dots, m$.

The functions $\mathfrak{a}(\omega)$, $\bar{\mathfrak{a}}(\omega)$ and $G(\omega, \xi)$ are transcendental and are defined as solutions of integral equations. Through these functions and through the ‘canonical contour’ C (see figure 1) the temperature and the magnetic field enter the multiple integral formula. The integral equation for $\mathfrak{a}(\omega)$ is non-linear,

$$\ln \mathfrak{a}(\lambda) = -\frac{h}{T} + \frac{2J}{\lambda(\lambda + i)T} - \int_C \frac{d\omega}{\pi} \frac{\ln(1 + \mathfrak{a}(\omega))}{1 + (\lambda - \omega)^2}, \quad (7)$$

and $\bar{\mathfrak{a}}(\omega) = 1/\mathfrak{a}(\omega)$ by definition. Looking at the free fermion limit $\Delta \rightarrow 0$ of the XXZ chain [15] it is natural to interpret the combinations $1/(1 + \mathfrak{a}(\omega))$ and $1/(1 + \bar{\mathfrak{a}}(\omega))$ as generalizations of the Fermi functions for holes and particles, respectively, to the interacting case.

The function $G(\omega, \xi)$ is related to the magnetization density. It satisfies the linear integral equation

$$G(\lambda, \xi) + \frac{1}{(\lambda - \xi)(\lambda - \xi - i)} = \int_C \frac{d\omega}{\pi(1 + a(\omega))} \frac{G(\omega, \xi)}{1 + (\lambda - \omega)^2}. \quad (8)$$

3 Reduction of multiple integrals

The multiple integrals (6) can be reduced by means of the integral equation (8). We demonstrate the method with the example $m = 2$ and then merely present our results for $m = 3$.

Emptiness formation probability for $m = 2$

Consider (6) for $m = 2$ and $\alpha_1 = \alpha_2 = \beta_1 = \beta_2 = 1$. Then

$$D_{11}^{11}(\xi_1, \xi_2)(\xi_2 - \xi_1) = \int_C \frac{d\omega_1}{2\pi(1 + a(\omega_1))} \int_C \frac{d\omega_2}{2\pi(1 + a(\omega_2))} \det(G(\omega_j, \xi_k)) \underbrace{\frac{(\omega_1 - \xi_1 - i)(\omega_2 - \xi_2)}{\omega_1 - \omega_2 - i}}_{=:r(\omega_1, \omega_2)}. \quad (9)$$

Here we may replace $r(\omega_1, \omega_2)$ by $[r(\omega_1, \omega_2) - r(\omega_2, \omega_1)]/2$, since the domain of integration of the double integral is symmetric. Now

$$r(\omega_1, \omega_2) - r(\omega_2, \omega_1) = \frac{(\omega_1 - \xi_1 - i)(\omega_2 - \xi_2)}{\omega_1 - \omega_2 - i} + \frac{(\omega_2 - \xi_1 - i)(\omega_1 - \xi_2)}{\omega_1 - \omega_2 + i} = \frac{P(\omega_1, \omega_2)}{1 + (\omega_1 - \omega_2)^2}, \quad (10)$$

and the polynomial $P(\omega_1, \omega_2)$ can be decomposed in such a way that

$$\frac{P(\omega_1, \omega_2)}{1 + (\omega_1 - \omega_2)^2} = \frac{p(\omega_1) - p(\omega_2)}{1 + (\omega_1 - \omega_2)^2} - \frac{2}{3}(\omega_1 - \omega_2) \quad (11)$$

with

$$p(\omega) = \frac{2}{3}\omega^3 - (\xi_1 + \xi_2 + i)\omega^2 + [i(\xi_1 + \xi_2 + \frac{i}{3}) + 2\xi_1\xi_2]\omega. \quad (12)$$

Then

$$D_{11}^{11}(\xi_1, \xi_2)(\xi_2 - \xi_1) = \frac{1}{4} \sum_{P \in \mathfrak{S}^2} \text{sign}(P) \int_C \frac{d\omega_1}{\pi(1 + a(\omega_1))} \frac{G(\omega_1, \xi_{P1})}{\pi(1 + a(\omega_2))} \int_C \frac{d\omega_2}{\pi(1 + a(\omega_2))} \left[\frac{p(\omega_1)}{1 + (\omega_1 - \omega_2)^2} - \frac{2}{3}\omega_1 \right]. \quad (13)$$

The second term in the square brackets on the right is already of factorized form. The first term can be reduced to factorized form by means of the integral equation (8). Finally

$$D_{11}^{11}(\xi_1, \xi_2)(\xi_1 - \xi_2) = \sum_{P \in \mathbb{G}^2} \text{sign}(P) \left[\frac{1}{12} (3\xi_{P1} - \xi_{P2} + i) \phi_1(\xi_{P1}) + \frac{1}{6} \phi_2(\xi_{P2}) - \frac{1}{6} \phi_1(\xi_{P1}) \phi_2(\xi_{P2}) - \frac{1}{24} (\xi_{P1} - \xi_{P2}) (1 + (\xi_{P1} - \xi_{P2})^2) \psi(\xi_{P1}, \xi_{P2}) \right], \quad (14)$$

where we have introduced a function

$$\psi(\xi_1, \xi_2) = \int_C \frac{d\omega}{\pi(1 + \mathfrak{a}(\omega))} \frac{G(\omega, \xi_1)}{(\omega - \xi_2)(\omega - \xi_2 - i)} \quad (15)$$

and a family of ‘moments’

$$\phi_j(\xi) = \int_C \frac{d\omega \omega^{j-1} G(\omega, \xi)}{\pi(1 + \mathfrak{a}(\omega))}, \quad j \in \mathbb{N}. \quad (16)$$

Note that $\psi(\xi_1, \xi_2)$ is symmetric. This can be shown by means of the integral equation (8). The physical meaning of $\psi(\xi_1, \xi_2)$ becomes evident in the limit of vanishing temperature and magnetic field, where it can be expressed in terms of gamma functions,

$$\lim_{T \rightarrow 0} \lim_{h \rightarrow 0} \psi(\xi_1, \xi_2) = 2i \partial_x \ln \left[\frac{\Gamma(\frac{1}{2} + \frac{ix}{2}) \Gamma(1 - \frac{ix}{2})}{\Gamma(\frac{1}{2} - \frac{ix}{2}) \Gamma(1 + \frac{ix}{2})} \right]_{x=\xi_1 - \xi_2}. \quad (17)$$

This is (up to a factor of -2) the two-spinon scattering phase [11, 19]. It plays an important role in the recent works [1, 2] as it is the only transcendental function entering the general formula for the density matrix at zero temperature and zero magnetic field. Instead of $\psi(\xi_1, \xi_2)$ we shall rather use the closely related expression

$$\gamma(\xi_1, \xi_2) = [1 + (\xi_1 - \xi_2)^2] \psi(\xi_1, \xi_2) - 1 \quad (18)$$

in terms of which our final formulae look neater. We also define $\lim_{h \rightarrow 0} \gamma(\xi_1, \xi_2) =: \gamma_0(\xi_1, \xi_2)$.

Considering the moments $\phi_j(\xi)$ in the same limit of zero temperature and magnetic field they turn into polynomials in ξ of order $j - 1$,

$$\lim_{T \rightarrow 0} \lim_{h \rightarrow 0} \phi_j(\xi) = \phi_j^{(0)}(\xi) = (-i\partial_k)^{j-1} \frac{2e^{ik\xi}}{1 + e^k} \Big|_{k=0}, \quad (19)$$

for instance,

$$\phi_1^{(0)}(\xi) = 1, \quad \phi_2^{(0)}(\xi) = \xi + \frac{i}{2}, \quad \phi_3^{(0)}(\xi) = \xi^2 + i\xi. \quad (20)$$

These polynomials satisfy the difference equation

$$\phi_j^{(0)}(\xi) + \phi_j^{(0)}(\xi - i) = 2\xi^{j-1}. \quad (21)$$

They allow us to define the ‘normalized moments’,

$$\varphi_j(\xi) = \phi_j(\xi) - \phi_j^{(0)}(\xi), \quad (22)$$

which vanish for $T, h \rightarrow 0$. We further introduce the symmetric combinations

$$\Delta_n(\xi_1, \dots, \xi_n) = \frac{\det(\varphi_j(\xi_k))|_{j,k=1,\dots,n}}{\prod_{1 \leq j < k \leq n} \xi_{kj}}, \quad (23)$$

with the shorthand notation $\xi_{kj} = \xi_k - \xi_j$.

The Δ_n will turn out to be particularly convenient for expressing the density matrix elements for $m = 2, 3$. Using Δ_1 and Δ_2 in (14) we obtain

$$D_{11}^{11}(\xi_1, \xi_2) = \frac{1}{4} + \frac{1}{4}(\Delta_1(\xi_1) + \Delta_1(\xi_2)) + \frac{1}{6}\Delta_2(\xi_1, \xi_2) - \frac{1}{12}\gamma(\xi_1, \xi_2). \quad (24)$$

The first moment φ_1 is exceptional among the φ_j in that it becomes trivial even for finite temperature if only the magnetic field vanishes,

$$\lim_{h \rightarrow 0} \varphi_1(\xi) = 0. \quad (25)$$

It follows that

$$\lim_{h \rightarrow 0} \Delta_j(\xi) = 0, \quad \text{for all } j \in \mathbb{N}. \quad (26)$$

Thus, for vanishing magnetic field,

$$D_{11}^{11}(\xi_1, \xi_2) = \frac{1}{4} - \frac{1}{12}\gamma_0(\xi_1, \xi_2) \quad (27)$$

and, in the homogeneous limit $\xi_1, \xi_2 \rightarrow 0$, we have rederived the result

$$\langle \sigma_1^z \sigma_2^z \rangle_{T, h=0} = 4D_{11}^{11}(T|0) - 1 = \frac{1}{3} - \lim_{h \rightarrow 0} \frac{1}{3} \int_C \frac{d\omega}{\pi(1 + \mathfrak{a}(\omega))} \frac{G(\omega, 0)}{\omega(\omega - i)} \quad (28)$$

for the nearest-neighbour two-point function which alternatively can be obtained [13] by taking the derivative of the free energy with respect to $1/T$. Here we can include the magnetic field into the calculation by simply taking the homogeneous limit in (24). We obtain

$$\langle \sigma_1^z \sigma_2^z \rangle_{T, h} = 4D_{11}^{11}(T|h) - 2\Delta_1(0) - 1 = \frac{2}{3}\Delta_2(0, 0) - \frac{1}{3}\gamma(0, 0) \quad (29)$$

which seems to be a new result. Note that the magnetic field not only enters through Δ_2 but also through γ . The homogeneous limit of Δ_n exists for all $n \in \mathbb{N}$ and is given by the formula

$$\lim_{\xi_n \rightarrow 0} \dots \lim_{\xi_1 \rightarrow 0} \Delta_n(\xi_1, \dots, \xi_n) = \det \left[\frac{\partial_{\xi}^{(k-1)} \varphi_j(\xi)}{(k-1)!} \right]_{\xi=0}. \quad (30)$$

Complete density matrix for $m = 2$

According to the rule $\alpha_1 + \alpha_2 = \beta_1 + \beta_2$ which reflects the conservation of S^z the density matrix for $m = 2$ has six non-vanishing elements. Using the Yang-Baxter algebra and certain identities of the type $D_1^1(\xi) + D_2^2(\xi) = 1$ we find four independent relations between the six non-vanishing elements,

$$\begin{aligned} D_{12}^{12}(\xi_1, \xi_2) &= D_1^1(\xi_1) - D_{11}^{11}(\xi_1, \xi_2), \quad D_{21}^{21}(\xi_1, \xi_2) = D_1^1(\xi_2) - D_{11}^{11}(\xi_1, \xi_2), \\ D_{22}^{22}(\xi_1, \xi_2) &= D_{11}^{11}(\xi_1, \xi_2) - D_1^1(\xi_1) - D_1^1(\xi_2) + 1, \\ D_{12}^{21}(\xi_1, \xi_2) - D_{21}^{12}(\xi_1, \xi_2) &= \frac{D_1^1(\xi_1) - D_1^1(\xi_2)}{i\xi_{12}}. \end{aligned} \quad (31)$$

Thus, we have to calculate one more independent linear combination, say $D_{12}^{21}(\xi_1, \xi_2) + D_{21}^{12}(\xi_1, \xi_2)$, in order to determine the complete density matrix for $m = 2$. The calculation can be done along the lines described above.

In order to obtain a convenient description of all density matrix elements we shall resort to a notation that we borrowed from [4][¶]. We arrange them into a column vector $h_m \in (\mathbb{C}^2)^{\otimes 2m}$ with coordinates labeled by $+$, $-$ instead of $1, 2$ according to the rule,

$$h_m^{\varepsilon_1, \dots, \varepsilon_m, \bar{\varepsilon}_m, \dots, \bar{\varepsilon}_1}(\lambda_1, \dots, \lambda_m) = D_{(3+\bar{\varepsilon}_1)/2, \dots, (3+\bar{\varepsilon}_m)/2}^{(3-\varepsilon_1)/2, \dots, (3-\varepsilon_m)/2}(\xi_1, \dots, \xi_m) \cdot \prod_{j=1}^m (-\bar{\varepsilon}_j), \quad (32)$$

where $\lambda_j = -i\xi_j$ for $j = 1, \dots, m$.

Then, setting $\mathbf{v}^t = (h_2^{++--}, h_2^{+-+-}, h_2^{+--+}, h_2^{-++-}, h_2^{-+-+}, h_2^{-++-})$,

$$\begin{aligned} \mathbf{v} &= \frac{1}{4}\mathbf{v}_0 - \frac{1}{12}\gamma(\xi_1, \xi_2)\mathbf{v}_1 \\ &\quad + \frac{1}{4}(\Delta_1(\xi_1) + \Delta_1(\xi_2))\mathbf{v}_2 - \frac{1}{4}(\Delta_1(\xi_1) - \Delta_1(\xi_2))\mathbf{v}_3 + \frac{1}{6}\Delta_2(\xi_1, \xi_2)\mathbf{v}_4 \end{aligned} \quad (33)$$

with

$$\begin{aligned} \mathbf{v}_0 &= (1, -1, 0, 0, -1, 1)^t, \\ \mathbf{v}_1 &= (1, 1, -2, -2, 1, 1)^t, \\ \mathbf{v}_2 &= (1, 0, 0, 0, 0, -1)^t, \\ \mathbf{v}_3 &= (0, 1, i\xi_{12}^{-1}, -i\xi_{12}^{-1}, -1, 0)^t, \\ \mathbf{v}_4 &= (1, 1, 1, 1, 1, 1)^t. \end{aligned} \quad (34)$$

From this we can read off the transverse neighbour correlation functions in a magnetic field to be $\langle \sigma_1^x \sigma_2^x \rangle_{T, h} = -\frac{1}{3}\Delta_2(0, 0) - \frac{1}{3}\gamma(0, 0)$.

[¶]This definition was first introduced in [2] and later modified in [4].

Emptiness formation probability for $m = 3$

As in the case $m = 2$ we can reduce the triple integral (6) representing the emptiness formation probability for $m = 3$ to sums over products of single integrals. Again we have to decompose the rational functions in the integrand appropriately and use the integral equation (8). It turns out that the final result can be represented in terms of the functions γ and Δ_j , $j = 1, 2, 3$,

$$\begin{aligned}
 D_{111}^{111}(\xi_1, \xi_2, \xi_3) = & \frac{1}{24} + \frac{1 + 5\xi_{12}\xi_{13}}{40\xi_{12}\xi_{13}}\Delta_1(\xi_1) + \frac{1 + 2\xi_{13}\xi_{23}}{24\xi_{13}\xi_{23}}\Delta_2(\xi_1, \xi_2) + \frac{1}{60}\Delta_3(\xi_1, \xi_2, \xi_3) \\
 & + \frac{1 - \xi_{13}\xi_{23}}{24\xi_{13}\xi_{23}}\gamma(\xi_1, \xi_2) - \frac{3 + 2\xi_{12}^2 + 5\xi_{13}\xi_{23}}{120\xi_{13}\xi_{23}}\gamma(\xi_1, \xi_2)\Delta_1(\xi_3) \\
 & + \text{cyclic permutations.} \quad (35)
 \end{aligned}$$

In the limit of vanishing magnetic field (26) applies and our result reduces to

$$D_{111}^{111}(\xi_1, \xi_2, \xi_3) = \frac{1}{24} + \frac{1 - \xi_{13}\xi_{23}}{24\xi_{13}\xi_{23}}\gamma_0(\xi_1, \xi_2) + \text{cyclic permutations.} \quad (36)$$

Note that the only effect of taking the limit $T \rightarrow 0$ is that the function $\gamma_0(\xi_1, \xi_2)$ changes into its zero temperature form (17), (18).

Complete density matrix for $m = 3$

We have factorized the full density matrix for $m = 3$. It contains 20 non-vanishing matrix elements, each of similar form to that in (35). Except for the emptiness formation probability D_{111}^{111} we also reduced the integrals for the symmetric combination $D_{121}^{112} + D_{211}^{121} + D_{121}^{211} + D_{211}^{112} + D_{112}^{121} + D_{112}^{211}$. Using relations similar to (31) and the high temperature expansion data for the inhomogeneous density matrix elements up to the order T^{-3} this was then enough to conjecture the complete density matrix for $m = 3$. We show it in a compact notation in the appendix. For our purposes here it is sufficient to know that all density matrix elements are linear combinations of the functions Δ_1 , Δ_2 , Δ_3 , γ and $\gamma\Delta_1$ with coefficients rational in the differences ξ_{jk} . For the case of vanishing magnetic field an ‘exponential formula’ for all density matrix elements is suggested in the next section.

The next-to-nearest neighbour two-point functions

It is a rather straightforward exercise to work out the next-to-nearest neighbour two-point functions from our general result for the $m = 3$ density matrix. We have to take

the appropriate linear combinations of density matrix elements and have to carry out the homogeneous limit $\xi_1, \xi_2, \xi_3 \rightarrow 0$. We obtain, for instance,

$$\begin{aligned} \langle \sigma_1^z \sigma_3^z \rangle_{T,h} &= \frac{2}{3} \Delta_2(0,0) - \frac{1}{3} \gamma(0,0) \\ &\quad - \frac{1}{6} (\Delta_2)_{xx}(0,0) + \frac{1}{3} (\Delta_2)_{xy}(0,0) - \frac{1}{6} \gamma_{xx}(0,0) + \frac{1}{3} \gamma_{xy}(0,0), \end{aligned} \quad (37a)$$

$$\begin{aligned} \langle \sigma_1^x \sigma_3^x \rangle_{T,h} &= -\frac{1}{3} \Delta_2(0,0) - \frac{1}{3} \gamma(0,0) \\ &\quad + \frac{1}{12} (\Delta_2)_{xx}(0,0) - \frac{1}{6} (\Delta_2)_{xy}(0,0) - \frac{1}{6} \gamma_{xx}(0,0) + \frac{1}{3} \gamma_{xy}(0,0). \end{aligned} \quad (37b)$$

Here we denoted derivatives with respect to the first and second argument, respectively, by subscripts x and y . Equations (37) generalize an important result of Takahashi [23] to include the temperature and the magnetic field.

4 The exponential formula

We observed in the previous section that for $m = 2, 3$ the density matrix for zero magnetic field is determined by a single transcendental function γ_0 (recall that $\lim_{h \rightarrow 0} \Delta_j = 0$). The situation is the same as for zero temperature. In fact, even the coefficients agree. Hence, it is tempting to substitute the function γ_0 for its zero temperature analogue into the general exponential formula recently obtained in [1]. This formula then gives the correct result for the 6 non-trivial density matrix elements for $m = 2$ and also for the emptiness formation probability and for the symmetric combination of density matrix elements mentioned in the previous section for $m = 3$. It further coincides up to order T^{-3} with the high-temperature expansion data for all 20 non-vanishing inhomogeneous density matrix elements for $m = 3$. For $m = 4$ we compared the conjectured form in the homogeneous case with the high-temperature expansion obtained from the homogeneous version [12, 14] of the multiple integral formula (6). For the emptiness formation probability we found full agreement up to the order of T^{-11} .

Conjecture 1. *The density matrix of a finite sub-chain of length m of the infinite XXX Heisenberg chain at finite T (for $h = 0$) is determined by the vector*

$$h_m(\lambda_1, \dots, \lambda_m) = \frac{1}{2^m} e^{\Omega_m^T(\lambda_1, \dots, \lambda_m)} \mathbf{s}_m, \quad \mathbf{s}_m = \prod_{j=1}^m s_{j, \bar{j}}, \quad (38)$$

$$\begin{aligned} \Omega_m^T(\lambda_1, \dots, \lambda_m) &= \frac{(-1)^{(m-1)}}{4} \int \int \frac{d\mu_1}{2\pi i} \frac{d\mu_2}{2\pi i} \frac{\gamma_0(i\mu_1, i\mu_2)(\mu_1 - \mu_2)}{[1 - (\mu_1 - \mu_2)^2]^2} \\ &\quad \times \text{tr}_{\mu_{1,2,2,2}} \left\{ T\left(\frac{\mu_1 + \mu_2}{2}; \lambda_1, \dots, \lambda_m\right) \otimes [T(\mu_1; \lambda_1, \dots, \lambda_m) \otimes T(\mu_2; \lambda_1, \dots, \lambda_m) \mathcal{P}^-] \right\}, \end{aligned} \quad (39)$$

through (32). By the integral over μ_1, μ_2 it is meant to take the residues at the poles $\lambda_1, \dots, \lambda_m$ of the integrand.

For the notation we are referring to [1]^{||}: The vector $s = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} - \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ is the spin singlet in $\mathbb{C}^2 \otimes \mathbb{C}^2$. The vector spaces in $(\mathbb{C}^2)^{\otimes 2m}$ are numbered in the order $1, 2, \dots, n, \bar{n}, \overline{n-1}, \dots, \bar{1}$. This defines \mathbf{s}_m . \mathcal{P}^- is the projector onto the one-dimensional subspace of $\mathbb{C}^2 \otimes \mathbb{C}^2$ spanned by s .

In order to define the transfer matrices in the integrand in (39) we first of all introduce an L -matrix $L(\lambda) \in U(\mathfrak{sl}_2) \otimes \text{End } \mathbb{C}^2$,

$$L(\lambda) = \frac{\rho(\lambda, d)}{2\lambda + d} (2\lambda + 1 + \Sigma^\alpha \otimes \sigma^\alpha), \quad (40)$$

where the $\Sigma^\alpha \in \mathfrak{sl}_2$ are a basis satisfying $[\Sigma^\alpha, \Sigma^\beta] = 2i\epsilon^{\alpha\beta\gamma}\Sigma^\gamma$, where d is determined by the Casimir element through $d^2 = (\Sigma^\alpha)^2 + 1$ and where $\rho(\lambda, d)$ satisfies the functional relation

$$\rho(\lambda, d)\rho(\lambda - 1, d) = \frac{2 - 2\lambda - d}{2\lambda - d} \quad (41)$$

(for more details see [1]). Then, for integer z , the ‘transfer matrices’

$$\begin{aligned} \text{tr}_z T(\lambda; \lambda_1, \dots, \lambda_n) = \\ \text{tr}_z L_{\bar{1}}(\lambda - \lambda_1 - 1) \dots L_{\bar{n}}(\lambda - \lambda_n - 1) L_n(\lambda - \lambda_n) \dots L_1(\lambda - \lambda_1) \end{aligned} \quad (42)$$

entering (39) are defined by substituting the irreducible representation of $U(\mathfrak{sl}_2)$ of dimension z into the definition (40) of the L -matrices. For non-integer z this can be analytically continued into the complex plane.

5 Discussion

Starting from the multiple-integral formula (6) we have investigated the density matrix of a finite segment of length m of the infinite isotropic Heisenberg chain at finite temperature and finite magnetic field. We found that the multiple integrals can be reduced to sums over products of single integrals, in much the same way as for $T, h = 0$. On the one hand this gives new efficient formulae for the calculation of finite-temperature short-range correlations of the XXX chain in the thermodynamic limit. On the other hand this shows that the density matrix and the correlation functions of the Heisenberg chain at finite temperature and finite magnetic field may be explored in a similar manner and to much the same extent as in the ground state case without magnetic field. When the magnetic field is switched off, but the temperature is kept finite the ‘algebraic

^{||}In fact, the only difference between our formula (38), (39) and the result of [1] is in the function γ_0 . In [1] a function ω was used which is related to γ_0 by

$$\omega(\lambda_1 - \lambda_2) = \lim_{T \rightarrow 0} \frac{\gamma_0(i\lambda_1, i\lambda_2)}{2(1 - (\lambda_1 - \lambda_2)^2)}.$$

structure' of the density matrix, as it shows up in the rational functions in the differences of the spectral parameters, seems to be still the same as for zero temperature, and only the 'physical part' of the expressions, encoded in the transcendental function γ_0 , changes. This is certainly true for $m \leq 2$ and for some of the density matrix elements for $m = 3$. From our high-temperature analysis it seems most likely true also for all density matrix elements for $m = 3, 4$, whence our conjecture 1 in the previous section. A second conjecture we are tempted to formulate inspecting our results for small m is the following: *In the case of non-vanishing magnetic field the density matrix elements for a segment of length m seem to depend only on γ and on $\Delta_1, \dots, \Delta_m$.*

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Appendix: Density matrix elements for $m = 3$

Here we show our result for other elements of the density matrix in the $m = 3$ case. We consider the 3 by 3 block

$$D_{3 \times 3} = \begin{pmatrix} D_{112}^{112} & D_{121}^{112} & D_{211}^{112} \\ D_{112}^{121} & D_{121}^{121} & D_{211}^{121} \\ D_{112}^{211} & D_{121}^{211} & D_{211}^{211} \end{pmatrix}. \quad (\text{A.1})$$

Another 3 by 3 block can be obtained from (A.1) by the substitution $1 \leftrightarrow 2$ and $h \rightarrow -h$. The answer looks as follows

$$\begin{aligned} D_{3 \times 3} = & A_0 + \sum_{1 \leq i < j \leq 3} A_{i,j} \gamma_{i,j} + \sum_{1 \leq i < j \leq 3; k \neq i,j} A_{i,j|k} \gamma_{i,j} \Delta_1(\xi_k) \\ & + \sum_{i=1}^3 B_i \Delta_1(\xi_i) + \sum_{1 \leq i < j \leq 3} B_{i,j} \Delta_2(\xi_i, \xi_j) + B_{1,2,3} \Delta_3(\xi_1, \xi_2, \xi_3), \end{aligned} \quad (\text{A.2})$$

where $\gamma_{i,j} = \gamma(\xi_i, \xi_j)$ and $A_0, A_{i,j}, A_{i,j|k}, B_i, B_{i,j}, B_{1,2,3}$ are 3 by 3 matrices. In order to define them let us introduce 3 by 3 matrices with the following elements

$$\begin{aligned} (e_0)_{k,l} = \delta_{k,l}, \quad (Z_0)_{k,l} = 1, \quad (X_i)_{k,l} = \begin{cases} -1 & \text{if } k = l = i \\ 1 & \text{if } k = l \neq i, \\ 0 & \text{otherwise} \end{cases} \\ X_{i,j}^{\pm} = e_i^j \pm e_j^i \quad \text{for } i < j, \quad (e_i^j)_{k,l} = \delta_{i,k} \delta_{j,l}, \quad 1 \leq i, j, k, l \leq 3. \end{aligned} \quad (\text{A.3})$$

We also define $X_{j,i}^{\pm} = X_{i,j}^{\pm}$ and $X_{i+3n} = X_i$, $X_{i+3n,j+3m}^{\pm} = X_{i,j}^{\pm}$ for $n, m \in \mathbb{Z}$. Then

$$\begin{aligned}
A_0 &= \frac{1}{8} e_0, \\
A_{i,j} &= -\frac{1}{24} \frac{1}{\xi_{ik} \xi_{jk}} (X_2 - 2X_{1,3}^+) + \frac{i}{24} \left(\frac{(-1)^j}{\xi_{ik}} + \frac{(-1)^i}{\xi_{jk}} \right) Y + \frac{1}{24} (X_{-j} - 2X_{-i,-k}^+), \\
Y &= X_{1,2}^- - X_{1,3}^- + X_{2,3}^-, \\
A_{i,j|k} &= \frac{1}{24} (e_0 - 2X_{-i,-k}^+) - \frac{1}{24} \frac{1}{\xi_{ik} \xi_{jk}} \left(\frac{2}{5} Z_0 - e_0 \right) + \frac{1}{24} \left(\frac{i}{\xi_{ik}} + \frac{i}{\xi_{jk}} \right) X_{1,3}^- \\
&\quad - \frac{1}{24} \frac{\xi_{ij}}{\xi_{ik}} \left(\frac{2}{5} Z_0 - X_{-j,-i}^+ - X_{-i,-k}^+ \right) + \frac{1}{24} \frac{\xi_{ij}}{\xi_{jk}} \left(\frac{2}{5} Z_0 - X_{-j,-k}^+ - X_{-i,-k}^+ \right). \tag{A.4}
\end{aligned}$$

$$\begin{aligned}
B_i &= \frac{1}{8} X_{-i+1} + \frac{1}{8} \frac{i}{\xi_{ij}} X_{-i,-k}^- + \frac{1}{8} \frac{i}{\xi_{ik}} X_{-j,-k}^- - \frac{1}{8} \frac{1}{\xi_{ij} \xi_{ik}} \left(\frac{1}{5} Z_0 - X_{1,3}^+ \right), \\
B_{i,j} &= -\frac{1}{12} (X_{-j} + X_{-i,-k}^+) - \frac{1}{24} \frac{1}{\xi_{ik} \xi_{jk}} (X_2 + X_{13}^+) \\
&\quad + \frac{1}{24} \frac{i}{\xi_{ik}} \left(2X_{-j,-k}^- - (-1)^k X_{-i,-j}^- - (-1)^i X_{-i,-k}^- \right) \\
&\quad + \frac{1}{24} \frac{i}{\xi_{jk}} \left(2X_{-i,-j}^- - (-1)^k X_{-j,-k}^- - (-1)^j X_{-i,-k}^- \right), \\
B_{1,2,3} &= -\frac{1}{20} Z_0. \tag{A.5}
\end{aligned}$$

It is implied in the above formulae that the triple (i, j, k) is always the cyclic permutation of $(1, 2, 3)$ and also that $A_{i,j} = A_{j,i}$, $A_{i,j|k} = A_{j,i|k}$, $B_{i,j} = B_{j,i}$. Let us also mention that the matrices A_0 and $A_{i,j}$ coincide with those which can be obtained from the formula (39).

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